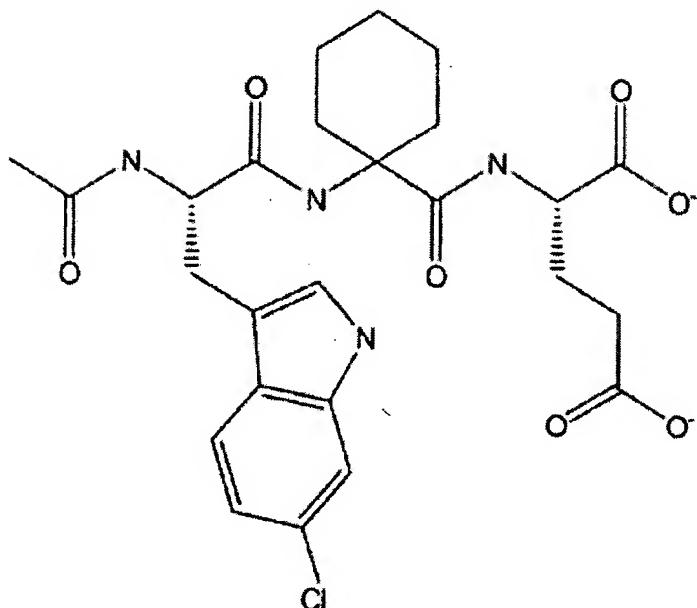


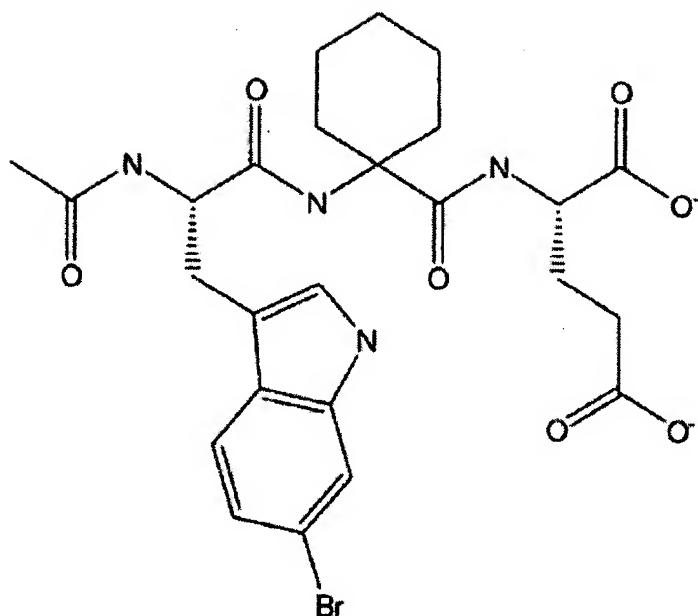
Steadman, David

From: Steadman, David
Sent: Friday, October 19, 2007 11:44 AM
To: STIC-EIC1600/2900
Subject: 10/822,254 structure search request

NAME: \ David Steadman
AU: 1656
Date: 10/19/07
Office: Remsen 2D11
Mailbox: Remsen 3C70

Please search the following two (2) structures in STN:





Thank you very much.

David

David J. Steadman, Ph.D.
Primary Examiner
Art Unit 1656
Protein Crystallography and Recombinant Enzymes
Office: Remsen 2B05
Mailbox: Remsen 3C70
Phone: (571) 272-0942

10/822254

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STRUCTURE FILE UPDATES: 18 OCT 2007 HIGHEST RN 950981-10-9
DICTIONARY FILE UPDATES: 18 OCT 2007 HIGHEST RN 950981-10-9

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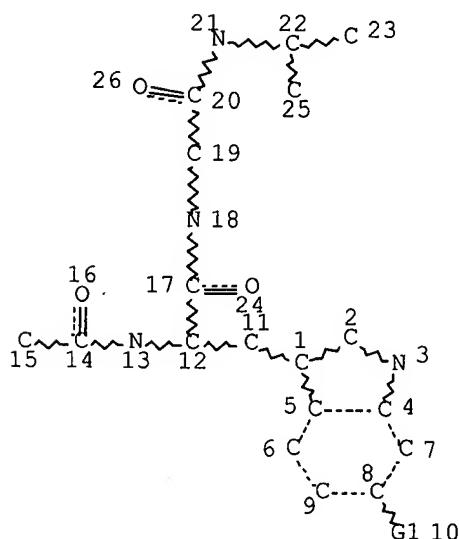
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<http://www.cas.org/support/stngen/stndoc/properties.html>

L1 STR



VAR G1=CL/BR

NODE ATTRIBUTES:

NSPEC IS R AT 19

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE

L3 2 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 418 ITERATIONS
 SEARCH TIME: 00.00.01

2 ANSWERS

FILE 'CAPLUS' ENTERED AT 14:47:49 ON 19 OCT 2007
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FILE COVERS 1907 - 19 Oct 2007 VOL 147 ISS 18
 FILE LAST UPDATED: 18 Oct 2007 (20071018/ED)

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L4 1 S L3

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:140668 CAPLUS Full-text
 DOCUMENT NUMBER: 142:235231
 TITLE: Soluble, stable form of human Double Minute 2 protein, hdm2, amenable to crystallization and use for structure-based drug design
 INVENTOR(S): Taremi, Shahriar Shane; Xie, Gaolian; Hesson, Thomas; Duca, Jose S.; Strickland, Corey; Windsor, William T.; Madison, Vincent S.; Zhang, Rumin; Reichert, Paul
 PATENT ASSIGNEE(S): Schering Corporation, USA
 SOURCE: U.S. Pat. Appl. Publ., 49 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|------------|
| US 2005037383 | A1 | 20050217 | US 2004-822254 | 20040409 |
| PRIORITY APPLN. INFO.: | | | US 2003-461787P | P 20030410 |
| | | | US 2004-547265P | P 20040224 |

AB The present invention relates to a soluble and stable form of human Double Minute 2 protein, Hdm2. The present invention further pertains to nucleic acids encoding these proteins. The present invention also relates to a process of obtaining specific samples of Hdm2 that are amenable to forming homogeneous crystals for x-ray crystallization anal. and the crystals formed thereby. The present invention also pertains to methods of using the x-ray

diffractable crystals in structure-based drug design to identify compds. that can modulate the activity of the protein. The present invention provides modified Hdm2 proteins that are amenable to crystallization and are soluble in E. coli exts. The present invention further discloses a set of amino acid substitutions of the Hdm2 protein that improve its solubility and/or stability without compromising its ability to bind p53. The present invention provides stable modified Hdm2 proteins produced by introducing an amino acid substitution into one or more of a unique set of amino acid residues of Hdm2. The modified Hdm2 proteins of the present invention have an improved solubility and form novel crystals that heretofore were unattainable with the wildtype Hdm2 protein. In addition, the present invention provides two specific ligands for Hdm2, the acetylated tripeptides, Ac-6ClWAC3cE and Ac-6BrWAC3cE. These tripeptides can be used to bind the modified Hdm2 proteins of the present invention to form a protein-ligand complex that is then crystallized. Such x-ray diffractable crystals can be used for structure based drug design to identify antitumor drugs.

IT 844901-80-0 844901-81-1

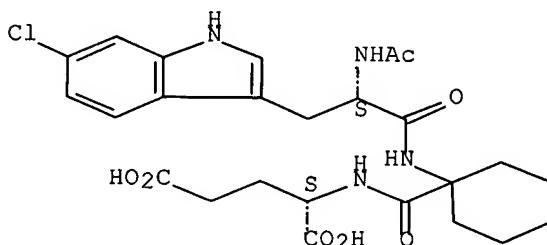
RL: BSU (Biological study, unclassified); NUU (Other use, unclassified); BIOL (Biological study); USES (Uses)

(modified Hdm2 protein complexed to; soluble, stable form of human Double Minute 2 protein, hdm2, amenable to crystallization and use for structure-based drug design)

RN 844901-80-0 CAPLUS

CN L-Glutamic acid, N-acetyl-6-chloro-L-tryptophyl-1-aminocyclohexanecarbonyl- (9CI) (CA INDEX NAME)

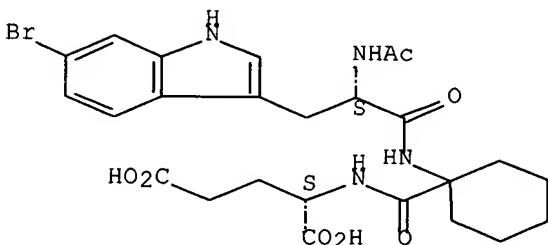
Absolute stereochemistry.



RN 844901-81-1 CAPLUS

CN L-Glutamic acid, N-acetyl-6-bromo-L-tryptophyl-1-aminocyclohexanecarbonyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



10/822254

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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L5 0 L3

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L6 0 L3

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FILE CONTENT: 1961-PRESENT VOL 147 ISS 16 (20071012/ED)

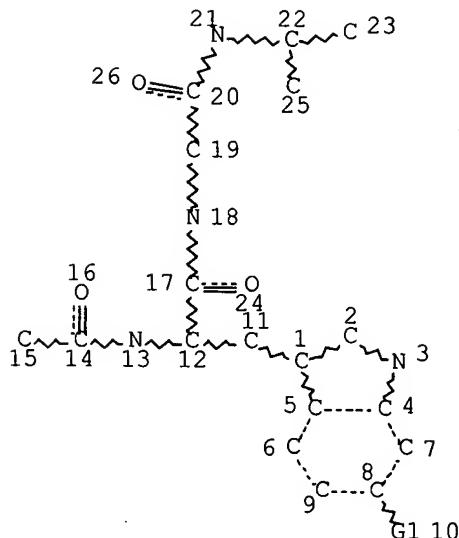
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MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

| | | |
|----|--------------|-------------|
| US | 2007207949 | 06 SEP 2007 |
| DE | 102006007895 | 30 AUG 2007 |
| EP | 1826829 | 29 AUG 2007 |
| JP | 2007221039 | 30 AUG 2007 |
| WO | 2007101371 | 13 SEP 2007 |
| GB | 2435041 | 15 AUG 2007 |
| FR | 2897532 | 24 AUG 2007 |
| RU | 2304584 | 20 AUG 2007 |
| CA | 2537669 | 24 AUG 2007 |

Expanded G-group definition display now available.

L1 STR



VAR G1=CL/BR

NODE ATTRIBUTES:

NSPEC IS R AT 19

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE

ATTRIBUTES SPECIFIED AT SEARCH-TIME:

ECLEVEL IS LIM ON ALL NODES

ALL RING(S) ARE ISOLATED

L8 1 SEA FILE=MARPAT SSS FUL L1 (MODIFIED ATTRIBUTES)

100.0% PROCESSED 3042 ITERATIONS
SEARCH TIME: 00.00.05

1 ANSWERS

FILE 'CAPLUS' ENTERED AT 14:49:04 ON 19 OCT 2007

L9 1 S L8

L10 1 S L9 NOT L4

FILE 'MARPAT' ENTERED AT 14:49:17 ON 19 OCT 2007

L11 1 S L10

L11 ANSWER 1 OF 1 MARPAT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:410915 MARPAT Full-textTITLE: Peptides for inhibiting mdm2 function and use for
anticancer and antiviral therapyINVENTOR(S): Han, Kyou-Hoon; Chi, Seung-Wook; Kim, Hyun-Jeong;
Lee, Si-Hyung; Ahn, Min-Jung; Kim, Do-Hyoung; Kim,
Jae-Sung; Park, Shin-AePATENT ASSIGNEE(S): Korea Research Institute of Bioscience and
Biotechnology, S. KoreaSOURCE: PCT Int. Appl., 71 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| WO 2005097820 | A1 | 20051020 | WO 2004-KR3494 | 20041229 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| KR 2005098766 | A | 20051012 | KR 2005-931 | 20050105 |

PRIORITY APPLN. INFO.: KR 2004-23565 20040406

AB The invention provides peptides for inhibiting mdm2 (mouse double minute 2).
 The invention also relates to the use of mdm2 inhibiting peptides for
 anticancer and antiviral therapy.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE
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L12 99 SEA ABB=ON PLU=ON ("TAREMI S"? OR "SHAHRIAR T"?)/AU
 L13 3600 SEA ABB=ON PLU=ON ("XIE G"? OR "GAOLIAN X"?)/AU

L14 62 SEA ABB=ON PLU=ON "HESSON T"?/AU
 L15 64 SEA ABB=ON PLU=ON "DUCA J"?/AU
 L16 492 SEA ABB=ON PLU=ON "STRICKLAND C"?/AU
 L17 208 SEA ABB=ON PLU=ON "WINDSOR W"?/AU
 L18 5291 SEA ABB=ON PLU=ON ("MADISON V"? OR "VINCENT M"?)/AU
 L19 19729 SEA ABB=ON PLU=ON "ZHANG R"?/AU
 L20 682 SEA ABB=ON PLU=ON "REICHERT P"?/AU
 L21 157099 SEA ABB=ON PLU=ON ("WANG Y"? OR "YAOLIN W"?)/AU
 L22 0 SEA ABB=ON PLU=ON L12 AND L13 AND L14 AND L15 AND L16
 AND L17 AND L18 AND L19 AND L20 AND L21
 L23 27 S L12 AND (L13-L21)
 L24 132 S L13 AND (L14-L21)
 L25 8 S L14 AND (L15-L21)
 L26 21 S L15 AND (L16-L21)
 L27 59 S L16 AND (L17-L21)
 L28 57 S L17 AND (L18-L21)
 L29 37 S L18 AND (L19-L21)
 L30 603 S L19 AND (L20 OR L21)
 L31 0 S L20 AND L21
 L32 121 S (L12-L31) AND (HDM2 OR (HDM OR DM OR DOUBLE MINUTE) (5A) ()
 L33 16 S L32 AND ?CRYST?
 L34 14 DUP REM L33 (2 DUPLICATES REMOVED)

L34 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2007:215609 CAPLUS Full-text
 DOCUMENT NUMBER: 147:282099
 TITLE: Effects of additive on the nanocrystalline Co-Ni alloy by jet electrodeposition
 AUTHOR(S): Wang, Nan; Jing, Tianfu; Qiao, Guiying; Wang, Yuhui; Yang, Jun
 CORPORATE SOURCE: Key Laboratory of Metastable Material Science and Technology, Material Science and Engineering College, Yanshan University, Qinhuangdao, 066004, Peop. Rep. China.
 SOURCE: Diandu Yu Huanbao (2006), 26(2), 7-10
 CODEN: DYHUEU; ISSN: 1000-4742
 PUBLISHER: Diandu Yu Huanbao Bianjibu
 DOCUMENT TYPE: Journal
 LANGUAGE: Chinese
 AB The nanocryst. Co-Ni alloys were prepared by jet electrodeposition in the nickel chloride and cobalt sulfate bath containing additive and the cathodic polarization curves of Co-Ni alloys were measured. Influence of additive on cathodic overpotential, current efficiency, the Co content, phase microstructure, grain size, microhardness, soft magnetic performance and surface morphol. of deposits were also investigated. The composition and technol. condition of Co-Ni alloy electrolyte comprises: CoSO₄·7H₂O 80g/L-, NiCl₂·6H₂O 200g/L-, H₃BO₃ 30g/L, benzosulfimide 0 and 2.5g/L, PH=4±0.1, J_k 51A·dm⁻², jet rate 5.52m/s, temperature of 40°C and time of 20min. Baths without any additive and with 2.5 g/L of additive are compared, the results show that the additive can increase cathodic overpotential and affect the kinetic process of Co and Ni electrodeposition. Cathodic overpotential increases from 3.594 V to 4.755 V, Co content and current efficiency have little change, but average grain size decreases from 12.8 nm to 5.5 nm, microhardness increases from Hv 423 to Hv 511, organic additive can improve the soft magnetic property of Co-Ni alloy.

L34 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 1
 ACCESSION NUMBER: 2005:140668 CAPLUS Full-text
 DOCUMENT NUMBER: 142:235231

TITLE: Soluble, stable form of human Double Minute 2 protein, **hdm2**, amenable to crystallization and use for structure-based drug design

INVENTOR(S): Taremi, Shahriar Shane; Xie, Gaolian; Hesson, Thomas; Duca, Jose S.; Strickland, Corey; Windsor, William T.; Madison, Vincent S.; Zhang, Rumin; Reichert, Paul

PATENT ASSIGNEE(S): Schering Corporation, USA

SOURCE: U.S. Pat. Appl. Publ., 49 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|------------|
| US 2005037383 | A1 | 20050217 | US 2004-822254 | 20040409 |
| PRIORITY APPLN. INFO.: | | | US 2003-461787P | P 20030410 |
| | | | US 2004-547265P | P 20040224 |

AB The present invention relates to a soluble and stable form of human Double Minute 2 protein, **Hdm2**.

The present invention further pertains to nucleic acids encoding these proteins. The present invention also relates to a process of obtaining specific samples of **Hdm2** that are amenable to forming homogeneous **crystals** for x-ray **crystallization** anal. and the **crystals** formed thereby. The present invention also pertains to methods of using the x-ray diffractable **crystals** in structure-based drug design to identify compds. that can modulate the activity of the protein. The present invention provides modified **Hdm2** proteins that are amenable to **crystallization** and are soluble in E. coli exts. The present invention further discloses a set of amino acid substitutions of the **Hdm2** protein that improve its solubility and/or stability without compromising its ability to bind p53. The present invention provides stable modified **Hdm2** proteins produced by introducing an amino acid substitution into one or more of a unique set of amino acid residues of **Hdm2**. The modified **Hdm2** proteins of the present invention have an improved solubility and form novel **crystals** that heretofore were unattainable with the wildtype **Hdm2** protein. In addition, the present invention provides two specific ligands for **Hdm2**, the acetylated tripeptides, Ac-6ClWAC3cE and Ac-6BrWAC3cE. These tripeptides can be used to bind the modified **Hdm2** proteins of the present invention to form a protein-ligand complex that is then **crystallized**. Such x-ray diffractable **crystals** can be used for structure based drug design to identify antitumor drugs.

L34 ANSWER 3 OF 14 MEDLINE on STN DUPLICATE 2

ACCESSION NUMBER: 2004052377 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 14753362

TITLE: Effect of alkali pretreatment of wheat straw on the efficacy of exogenous fibrolytic enzymes.

AUTHOR: Wang Y; Spratling B M; ZoBell D R; Wiedmeier R D; McAllister T A

CORPORATE SOURCE: Agriculture and Agri-Food Canada Research Centre, Lethbridge, Alberta, T1J 4B1 Canada.

SOURCE: Journal of animal science, (2004 Jan) Vol. 82, No. 1, pp. 198-208.

PUB. COUNTRY: Journal code: 8003002. ISSN: 0021-8812.
 DOCUMENT TYPE: United States
 (Journal; Article; (JOURNAL ARTICLE)
 (RESEARCH SUPPORT, NON-U.S. GOV'T)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 200408
 ENTRY DATE: Entered STN: 3 Feb 2004
 Last Updated on STN: 7 Aug 2004
 Entered Medline: 6 Aug 2004

AB The effects of pretreating wheat straw with alkali on the efficacy of exogenous fibrolytic enzymes for improving straw digestibility were studied in vitro, in situ, and in vivo. In Exp. 1, untreated straw (US); alkali-treated (5% NaOH, wt/wt) straw (AS); and autoclaved, alkali-treated straw (AAS) were sprayed with 0 or 1.5 mg/g DM of enzyme mix (xylanase, beta-glucanase, carboxymethylcellulase, and amylase) and incubated for 30 h in buffered ruminal fluid (3 x 2 factorial arrangement). Enzymes increased ($P < 0.001$) gas production and the incorporation of ^{15}N into microbial N at 4 h, more so with AS or AAS than with US ($P < 0.001$ for gas; $P < 0.05$ for ^{15}N). In Exp. 2, US and AS were sprayed with enzymes at 0, 0.15, or 1.5 mg/g DM (2 x 3 factorial) and incubated ruminally in nylon bags for up to 80 h to determine the in situ DM disappearance (ISDMD). Interactive effects ($P < 0.05$) of pretreatment and enzymes were observed on all ruminal degradation parameters. Alkali increased the rate ($P < 0.01$) and extent ($P < 0.001$) of ISDMD irrespective of enzymes. Enzymes applied to US did not affect the extent of ISDMD, but they increased ($P < 0.01$) the extent of ISDMD when applied to AS. Substrates from Exp. 1 and 2 were incubated in acetate buffer for 24 h to measure the hydrolytic loss of DM and release of reducing sugars and phenolic compounds. Alkali pretreatment and enzymes each increased ($P < 0.001$) DM loss and the release of reducing sugars and, in combination, exerted synergistic effects ($P < 0.001$). Enzymes did not affect the release of phenolic compounds from the straw. In Exp. 3, total-tract digestibility of untreated and enzyme-treated (100 mL/kg DM) ammoniated straw was assessed using 32 beef cows in eight pens. Wrapped straw bales were injected with NH₃ (3% [wt/wt], DM basis) 4 mo before the study; enzymes were applied immediately before feeding. Applying enzyme to ammoniated straw increased ($P < 0.05$) digestibilities of DM, OM, and total N but did not affect the intake of DM or digestibility of ADF. Pretreatment of straw with alkali enhanced the efficacy of exogenous enzymes, presumably by breaking esterified bonds and releasing phenolic compounds and/or by swelling the **crystalline** cellulose and enhancing enzyme penetration. Including enzymes that mimic alkali hydrolysis (e.g., esterases) in commercial feed additives could substantially improve the value of these products for ruminants.

L34 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:202295 CAPLUS Full-text
 DOCUMENT NUMBER: 141:270331
 TITLE: Synthesis, **crystal** structure and
 nonlinear optical properties of a cluster compound
 containing the bipy ligand
 AUTHOR(S): Zhou, Jian-Liang; Li, Yi-Zhi; Zheng, He-Gen; Xin,
 Xin-Quan; Yin, Tao; Wang, Yu-Xiao; Song,
 Ying-Lin
 CORPORATE SOURCE: Coordination Chemistry Institute, State Key
 Laboratory of Coordination Chemistry, Nanjing
 University, Nanjing, 210093, Peop. Rep. China
 SOURCE: Transition Metal Chemistry (Dordrecht,
 Netherlands) (2004), 29(2), 185-188
 CODEN: TMCHDN; ISSN: 0340-4285

PUBLISHER: Kluwer Academic Publishers
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 141:270331

AB The [MoO_{0.75}S_{3.25}Cu₃Cl(bipy)₂] complex was synthesized for nonlinear optical studies by the reaction of (NH₄)₂[MoOS₃], CuCl and bipy in CH₂Cl₂ solution. A single crystal x-ray anal. revealed that the complex consists of a nest-shaped core. The Mo atom is tetrahedrally coordinated by four S atoms, or three S atoms and one terminal O atom. There are two types of copper atom in the MoO_{0.75}S_{3.25}Cu₃ aggregate: two copper atoms are tetrahedrally coordinated and another copper atom is trigonally coordinated. The 3rd-order nonlinear optical properties were studied by the Z-scan technique with 8 ns laser pulses at 532 nm. The cluster exhibits both optical self-focusing and optical nonlinear absorption (effectively $n_2 = 1.3 + 10^{-11}$ e s u., $\alpha_2 = 1.2 + 10^{-10}$ m W⁻¹ in a 2.68×10^{-4} mol dm⁻³ CH₂Cl₂ solution).

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2003:201695 CAPLUS Full-text
 DOCUMENT NUMBER: 140:11958
 TITLE: Synthesis, crystal structure and non-linear optical properties of the heterobimetallic polymeric compound {[n-Bu₄N][W₂Ag₃S₈]}_n
 AUTHOR(S): Zhou, Jian-Liang; Wang, Yu-Xiao; Wang, Yan; Song, Ying-Lin; Zheng, He-Gen; Li, Yi-Zhi; Yang, Lan-Ping; Xin, Xin-Quan
 CORPORATE SOURCE: State Key Laboratory of Coordination Chemistry, Coordination Chemistry Institute, Nanjing University, Nanjing, 210093, Peop. Rep. China
 SOURCE: CrystEngComm (2003), 5, 62-64
 CODEN: CRECF4; ISSN: 1466-8033
 URL: <http://www.rsc.org/CFCart/displayarticleonfr ee.cfm?article=8%2D9%223%24%5DVZB%214%2E%5FL1%286%2COZ5%3D87PE%40%3D29%23%3C%0A>

PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal; (online computer file)
 LANGUAGE: English

AB The heterobimetallic, polymeric compound was synthesized by the reaction of (NH₄)₂WS₄ and AgBr with Bu₄NBr in CH₂Cl₂ solution under a purified nitrogen atmospheric using standard Schlenk techniques. The crystals were characterized by elemental anal., IR and single-crystal x-ray crystallog. The polymeric anion has a hanging ladder-like polymeric chain which can also be described as double helical chains bridged by silver atoms. Its nonlinear optical properties (NLO) were investigated using Z-scan techniques with an 8 ns pulsed laser at 532 nm, and the cluster also exhibits both strong nonlinear optical absorption and an optical self-defocusing effect (effective $\alpha_2 = 1.11 \times 10^{-10}$ m W⁻¹, $n_2 = 3.67 \times 10^{-18}$ m² W⁻¹, when measured with a 1.2×10^{-4} mol dm⁻³ DMF suspension).

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2001:764391 CAPLUS Full-text
 DOCUMENT NUMBER: 136:69890
 TITLE: Synthesis, structure and optical refractive effect of dibutyltin(IV) complex of [Ph₂P(S)NP(S)Ph₂]⁻

AUTHOR(S): Niu, Yunyin; Wang, Yuxiao; Song, Yinglin; Liu, Shixiong; Zheng, Hegen; Xin, Xinquan
 CORPORATE SOURCE: State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing, 210093, Peop. Rep. China
 SOURCE: Chemistry Letters (2001), (10), 1004-1005
 CODEN: CMLTAG; ISSN: 0366-7022
 PUBLISHER: Chemical Society of Japan
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:69890
 AB Reaction of Bu₂SnCl₂ with K[Ph₂P(S)NP(S)Ph₂] in MeCN gives the spirobimetalallocyclic complex bis(tetraphenyldithioimidodiphosphinato)dibutyltin(IV), {Bu₂Sn[Ph₂P(S)N-P(S)Ph₂]₂} in which π-π stacking interactions by the Ph rings of the ligands exist. The nonlinear optical (NLO) properties were studied with an 8 ns-pulsed laser at 532 nm. Its optical responses to the incident light exhibit strong refractive effect with n₂ = 5.4 + 10⁻¹⁸ m² W⁻¹ in a 1.2 + 10⁻⁴ mol dm⁻³ DMF solution
 REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2000:541980 CAPLUS Full-text
 DOCUMENT NUMBER: 133:316762
 TITLE: Studies on two interesting microporous polymeric clusters {[Et₄N]₂[MS₄Cu₄(CN)₄]}_n (M = Mo or W) with three-dimensional open frameworks: synthesis, structural characterization, strong optical non-linearities and large optical limiting properties
 AUTHOR(S): Zhang, Chi; Song, Yinglin; Xu, Yan; Fun, Hoongkun; Fang, Guangyu; Wang, Yuxiao; Xin, Xinquan
 CORPORATE SOURCE: Department of Physics, State Key Laboratory of Applied Optics, Harbin Institute of Technology, Harbin, 150001, Peop. Rep. China
 SOURCE: Dalton (2000), (16), 2823-2829
 CODEN: DALTFG; ISSN: 1470-479X
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Reactions combining stoichiometric amts. of (Et₄N)₂MS₄ (M = Mo or W) and CuCN (1:4) in pyridine afforded interesting three-dimensional cluster polymers with open frameworks {[Et₄N]₂[MS₄Cu₄(CN)₄]}_n [M = Mo (1) or W (2)]. Crystal structure determination shows that the anionic MS₄Cu₄ units bridged by cyanide produce three-dimensional channels running down the crystallog. a axis. An alternative way to view this framework is in terms of the diamond structure, where C has alternately been replaced by a MS₄Cu₄ aggregate and C-C by two parallel cyanide bridging ligands. In these intersecting channels the shortest distances between Cu atoms along the b and c axes are 15.22 and 8.11 Å, resp.. Non-linear optical properties of the two clusters were studied first with an 8 ns pulsed laser at 532 nm. These two clusters exhibit large optical limiting performance with limiting threshold values of 0.28 for 1, 0.15 J cm⁻² for 2 resp. Both compds. show strong third-order NLO absorption effects (α^2 1.5 + 10⁻⁹ 1, 1.6 + 10⁻⁹ m W⁻¹ 2) and self-focusing performance (n₂ 1.84 + 10⁻¹⁶ 1, 1.22 + 10⁻¹⁶ m² W⁻¹ 2) in 3.64 + 10⁻⁵ 1 and 2.93 + 10⁻⁵ mol dm⁻³ 2 DMF solution sep. The corresponding effective NLO susceptibilities $\chi(3)$ are 4.58

+ 10-9 1 and 5.12 + 10-9 esu 2 while the corresponding hyperpolarizabilities ($\gamma(1) = 1.15 + 10-29$ and $\gamma(2) = 1.26 + 10-29$ esu) are also reported.

REFERENCE COUNT: 81 THERE ARE 81 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2001:186215 CAPLUS Full-text
 DOCUMENT NUMBER: 134:320167
 TITLE: Two interesting heterobimetallic compounds [MOS₃Cu₃(4-pic)₆]·Br (M = Mo, W) with cationic cluster: synthesis, structural characterization, non-linear response and large optical limiting properties
 AUTHOR(S): Zhang, Chi; Song, Yinglin; Xu, Yan; Jin, Guocheng; Fang, Guangyu; Wang, Yuxiao; Fan, Hoongkun; Xin, Xinquan

CORPORATE SOURCE: Physical Department, Harbin Institute of Technology, Harbin, 150001, Peop. Rep. China
 SOURCE: Inorganica Chimica Acta (2000), 311(1-2), 25-32
 CODEN: ICHAA3; ISSN: 0020-1693

PUBLISHER: Elsevier Science S.A.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:320167

AB Two heterobimetallic cluster compds. [MOS₃Cu₃(4-pic)₆]·Br (M = Mo 1, W 2) with cationic cluster skeleton and halide anion Br⁻ synthesized by the reaction of (NH₄)₂MOS₃, CuBr and 4-picoline (4-pic) are presented. Their structures were crystallog. determined and such nest-shaped cationic clusters, obtained for the 1st time, are interesting in comparison with the analogical nest-shaped clusters with a neutral skeleton or anionic skeleton. The nonlinear optical (NLO) properties of these two clusters were studied with an 8 ns pulsed laser at 532 nm. These two clusters exhibit large optical limiting abilities with limiting thresholds F_{th} = 0.18 J cm⁻² (1) and F_{th} = 0.15 J cm⁻² (2), resp. Both compds. show strong 3rd-order NLO absorption effects (α_2 -value of 1.6 + 10-10 m W-1 1, 2.8 + 10-10 m W-1 2) and self-focusing performance (n_2 -value of 4.56 + 10-11 esu 1, 4.62 + 10-11 esu 2) in 3.86 + 10-4 mol dm⁻³ 1 and 8.89 + 10-4 mol dm⁻³ 2 DMF solution sep. The corresponding effective NLO susceptibilities $\chi(3)$ are 5.4 + 10-12 esu 1 and 5.5 + 10-12 esu 2 while the corresponding hyperpolarizabilities ($\gamma(1) = 2.51 + 10-31$ esu and $\gamma(2) = 1.03 + 10-31$ esu) are also reported.

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2000:60270. CAPLUS Full-text
 DOCUMENT NUMBER: 132:112360
 TITLE: Comprehensive utilization of waste residue from cefotaxime sodium production
 AUTHOR(S): Liu, Huiling; Zhou, Ding; Yue, Tongming; Zhao, Huihong; Wang, Yan
 CORPORATE SOURCE: Harbin Institute of Technology, Harbin, 150001, Peop. Rep. China
 SOURCE: Huanjing Wuran Yu Fangzhi (1999), 21(6), 17-19
 CODEN: HWYFEW; ISSN: 1001-3865
 PUBLISHER: Huanjing Wuran Yu Fangzhi Bianjibu
 DOCUMENT TYPE: Journal
 LANGUAGE: Chinese

AB A process for recovering 2-mercaptopbenzothiazole (M) with waste residue from cefotaxime sodium production and synthesizing 2, 2-dibenzothiazolyl disulfide (DM) was developed, which comprises impregnating the waste residue in 2M Na₂CO₃ at 60° for 0.5 h, filtrating, adjusting pH to 3.5 with 2M H₂SO₄, filtrating, drying, dissolving the obtained coarse M in ethanol, recrystg. to obtain refined M, reacting the refined M with 3.5% NaNO₂ at 60° with addition of 2.5% H₂SO₄ and introduction of air, and drying to obtain DM. The yield of DM reached 23.8%.

L34 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1995:247642 CAPLUS Full-text
 DOCUMENT NUMBER: 122:119568
 TITLE: Two heterocyclic 1,2,4,5-tetrazines
 AUTHOR(S): Yeh, Mou-Yung; Huang, Chun-Yin; Ueng, Chuen-Her;
 Wang, Yu
 CORPORATE SOURCE: Dep. Chem., Natl. Cheng Kung Univ., Tainan, Taiwan
 SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications (1994), C50(11), 1781-4
 CODEN: ACSCEE; ISSN: 0108-2701

PUBLISHER: Munksgaard
 DOCUMENT TYPE: Journal
 LANGUAGE: English

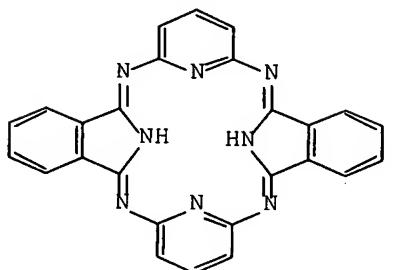
AB The title compds. 6-bromo-1,4-dihydro-1,4-di(o-tolyl)-1,2,4,5-tetrazin-3(2H)-one (I) and 3,6-dibromo-1,4-dihydro-1,4-bis(p-methoxyphenyl)-1,2,4,5-tetrazine (II) were prepared from 4-bromo-3-(o-tolyl)sydnone and 4-bromo-3-(p-methoxyphenyl)sydnone, resp., in THF under ultrasonic irradiation, and identified with IR, NMR, mass spectrum and elemental analyses. I is triclinic, space group P.hivin.1, with a 8.217(3), b 8.477(5), c 12.045(3) Å, 99.16(3), β 104.23(2), and γ 95.41(5)°; Z = 2, dc = 1.50, dm = 1.51(3); R = 0.044, Rw = 0.026 for 1937 reflections. II is orthorhombic, space group Pbcn, with a 18.975(3), b 10.327(2), and c 8.569(3) °; Z = 4, dc = 1.80, dm = 1.79(3); R = 0.037, Rw = 0.028 for 875 reflections. Atomic coordinates are given. The heterocyclic rings of both compds. appear to lack aromatic character, as judged from the bond lengths.

L34 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1987:487600 CAPLUS Full-text
 DOCUMENT NUMBER: 107:87600
 TITLE: Structures of 4-acetyl-3-(p-tolyl)sydnone (1) and 4-acetyl-3-phenylsydnone oxime (2)
 AUTHOR(S): Ueng, Chuen Her; Wang, Y.; Yeh, Mou Yung
 CORPORATE SOURCE: Dep. Chem., Natl. Taiwan Univ., Taipei, Taiwan
 SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications (1987), C43(6), 1122-5
 CODEN: ACSCEE; ISSN: 0108-2701

DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Title compound 1 is orthorhombic, space group P212121, with a 10.995(4), b 15.158(2), and c 6.530(3) Å; dm = 1.3(1) and dc = 1.33 for Z = 4; final R = 0.038 for 855 reflections. Title compound 2 is monoclinic, space group P21/n, with a 7.871(1), b 7.741(2), c 16.880(5) Å, and β 96.20(2)°; dm = 1.4(1) and dc = 1.42 for final R = 0.041 for 1553 reflections. Atomic coordinates are given. The bond lengths of the sydnone ring are similar in both structures. The bond lengths N(1)-C(7) and C(7)-C(8) of 3,4-disubstituted sydnone derivs. are longer than the corresponding bond lengths in 3-substituted sydnone derivs., and the dihedral angles between the sydnone ring and the Ph ring of compds. 1 and 2 (68.4(2) and 78.6(1)°, resp.) are larger than those of 3-substituted sydnone derivs. This may be attributed to steric effects.

L34 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1986:616975 CAPLUS Full-text
 DOCUMENT NUMBER: 105:216975
 TITLE: Structural relationships between the
 hemiporphyrazine macrocyclic ligand and its metal
 complexes. I. Saddle shaped neutral ligand
 hydrate, C₂₆H₁₆N₈·H₂O, and nickel complex,
 [Ni(C₂₆H₁₄N₈)]
 AUTHOR(S): Peng, Shie Ming; Wang, Yu; Ho, Tsang
 Feng; Chang, I Chen; Tang, Chia Pin; Wang, Chiung
 Jane
 CORPORATE SOURCE: Dep. Chem., Natl. Taiwan Univ., Taipei, 107,
 Taiwan
 SOURCE: Journal of the Chinese Chemical Society (Taipei,
 Taiwan) (1986), 33(1), 13-21
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The title hydrated ligand I orthorhombic, space group Pnmm, with a 4.6142(3),
 b 14.7687(7), and c 15.0650(5) Å; $\text{dm} = 1.46(2)$ and $\text{dc} = 1.48$ for $Z = 2$. The
 final $R = 0.068$ and $Rw = 0.038$. Ni(C₂₆H₁₄N₈) is monoclinic, space group I2/c,
 with a 22.0437(11), b 3.7637(4), c 23.4742(11) Å, and $\beta = 92.7(1)^\circ$; $\text{dm} = 1.68(2)$
 and $\text{dc} = 1.70$ for $Z = 4$. The final $R = 0.039$ and $Rw = 0.025$. The overall
 conformations of I and the Ni complex are similar, both have a pronounced
 saddle shape. The Ni-N bond distances are 1.861(2) and 1.998(2) Å. The
 distances from N atoms to the center of the ring in I are 2.020(3) and
 2.220(3) Å, which are significantly longer than those of Ni complex. A
 detailed comparison about the core size with similar ligand is presented.
 Atomic coordinates are given.

L34 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1985:551318 CAPLUS Full-text
 DOCUMENT NUMBER: 103:151318
 TITLE: The crystal structure of lanthanum
 rhodium boride (La_{1-x}Rh₃B₂)
 AUTHOR(S): Ku, H. C.; Ma, L. J.; Tai, M. F.; Wang, Y.
 ; Horng, H. E.
 CORPORATE SOURCE: Dep. Phys., Natl. Tsing Hua Univ., Hsinchu, 300,
 Taiwan
 SOURCE: Journal of the Less-Common Metals (1985), 109(2),

219-28

CODEN: JCOMAH; ISSN: 0022-5088

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB The crystal structure of La_{1-x}Rh₃B₂ was determined by single-crystal x-ray anal. La_{0.81}Rh₃B₂ crystallized in hexagonal space group P6/mmm, with a 5.642(1) and c 8.546(2) Å; d_m = 9.49 and d_c = 9.37 for Z = 3. The structure was refined by full-matrix least squares to R = 0.054 for 536 reflections. The crystal structure is a disordered superstructure (vacancy distorted) of the LaRh₃B₂ phase with the CeCo₃B₂-type structure (a 5.480 and c 3.137 Å). The coordination nos. of La are (1.6La) + 12Rh + 6B and those of Rh atoms (3.2La) + 6Rh + 4B. The isolated B atoms have tetrakaidecahedral metal coordination (2.4La) + 6Rh; no B-B contact occurs. Four new ternary Rh borides with this disordered La_{1-x}Rh₃B₂-type structure are reported with the general formula RE_{1-x}Rh₃B₂ (x = 0.5; RE = La, Ce, Pr, or Nd). The relation between structural chemical and phys. properties (supercond., ferromagnetism, valence fluctuation) is discussed.

L34 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1984:638436 CAPLUS Full-text

DOCUMENT NUMBER: 101:238436

TITLE: Reinvestigation of the structure of potassium pyrosulfite, K₂S₂O₅

AUTHOR(S): Chen, I Chia; Wang, Yu

CORPORATE SOURCE: Dep. Chem., Natl. Taiwan Univ., Taipei, Taiwan

SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications (1984), C40(11), 1780-1
CODEN: ACSCEE; ISSN: 0108-2701

DOCUMENT TYPE: Journal

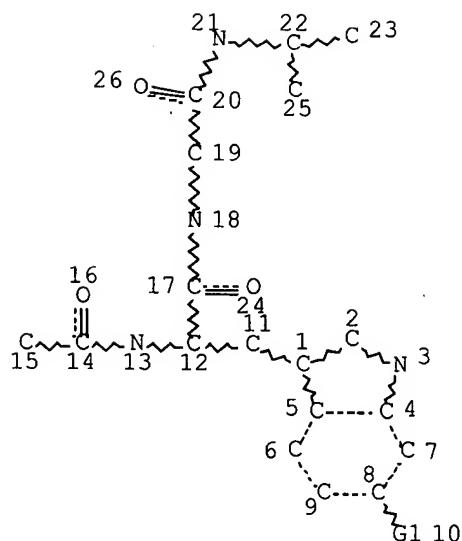
LANGUAGE: English

AB K₂S₂O₅ is monoclinic, space group P21/m, with a 6.921(1), b 6.160(1), c 7.537(1) Å, and β 102.79(1) $^\circ$; d_m = 2.36 and d_c = 2.356 for Z = 2. The final R = 0.040 for 780 reflections. The mol. contains a plane symmetry (S-S-O) and a long S-S bond (2.2194(9) Å) between the thionite and thionate groups. The S-O distances are 1.4870(8) Å in the thionite group and 1.453(1) and 1.4602(8) Å in the thionate group. A comparison with other compds. containing the S₂O₅²⁻ ion is made. Atomic coordinates are given.

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L1

STR



VAR G1=CL/BR

NODE ATTRIBUTES:

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DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

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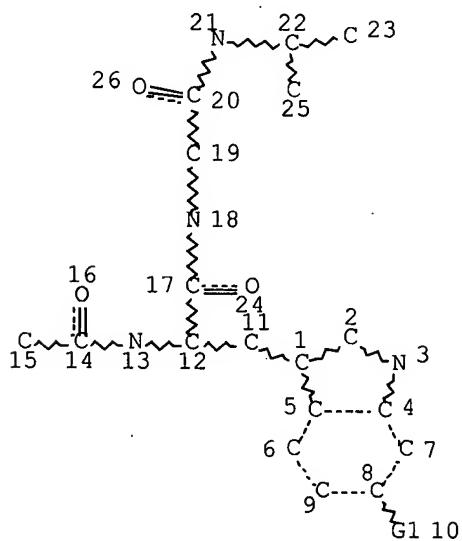
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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE

ATTRIBUTES SPECIFIED AT SEARCH-TIME:
 ECLEVEL IS LIM ON ALL NODES
 ALL RING(S) ARE ISOLATED

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 D SCAN
 D QUE
 L3 2 SEA SSS FUL L1
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 L4 1 SEA ABB=ON PLU=ON L3
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 D QUE STAT L3
 FILE 'CAPLUS' ENTERED AT 14:47:49 ON 19 OCT 2007
 D IBIB ABS HITSTR
 FILE 'CAOLD' ENTERED AT 14:47:49 ON 19 OCT 2007
 L5 0 SEA ABB=ON PLU=ON L3
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 L6 0 SEA ABB=ON PLU=ON L3
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 L7 0 SEA SSS SAM L1 (MODIFIED ATTRIBUTES)
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 L9 1 SEA ABB=ON PLU=ON L8
 L10 1 SEA ABB=ON PLU=ON L9 NOT L4
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 L11 1 SEA ABB=ON PLU=ON L10
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 L13 3600 SEA ABB=ON PLU=ON ("XIE G"? OR "GAOLIAN X"?)/AU
 L14 62 SEA ABB=ON PLU=ON "HESSON T"?/AU
 L15 64 SEA ABB=ON PLU=ON "DUCA J"?/AU
 L16 492 SEA ABB=ON PLU=ON "STRICKLAND C"?/AU

10/822254

L17 208 SEA ABB=ON PLU=ON "WINDSOR W"?/AU
L18 5291 SEA ABB=ON PLU=ON ("MADISON V"? OR "VINCENT M"?)/AU
L19 19729 SEA ABB=ON PLU=ON "ZHANG R"?/AU
L20 682 SEA ABB=ON PLU=ON "REICHERT P"?/AU
L21 157099 SEA ABB=ON PLU=ON ("WANG Y"? OR "YAOLIN W"?)/AU
L22 0 SEA ABB=ON PLU=ON L12 AND L13 AND L14 AND L15 AND L16
 AND L17 AND L18 AND L19 AND L20 AND L21
L23 27 SEA ABB=ON PLU=ON L12 AND ((L13 OR L14 OR L15 OR L16 OR
 L17 OR L18 OR L19 OR L20 OR L21))
L24 132 SEA ABB=ON PLU=ON L13 AND ((L14 OR L15 OR L16 OR L17 OR
 L18 OR L19 OR L20 OR L21))
L25 8 SEA ABB=ON PLU=ON L14 AND ((L15 OR L16 OR L17 OR L18 OR
 L19 OR L20 OR L21))
L26 21 SEA ABB=ON PLU=ON L15 AND ((L16 OR L17 OR L18 OR L19 OR
 L20 OR L21))
L27 59 SEA ABB=ON PLU=ON L16 AND ((L17 OR L18 OR L19 OR L20 OR
 L21))
L28 57 SEA ABB=ON PLU=ON L17 AND ((L18 OR L19 OR L20 OR L21))
L29 37 SEA ABB=ON PLU=ON L18 AND ((L19 OR L20 OR L21))
L30 603 SEA ABB=ON PLU=ON L19 AND (L20 OR L21)
L31 0 SEA ABB=ON PLU=ON L20 AND L21
L32 121 SEA ABB=ON PLU=ON ((L12 OR L13 OR L14 OR L15 OR L16 OR
 L17 OR L18 OR L19 OR L20 OR L21 OR L22 OR L23 OR L24 OR
 L25 OR L26 OR L27 OR L28 OR L29 OR L30 OR L31)) AND (HDM2
 OR (HDM OR DM OR DOUBLE MINUTE) (5A) (2 OR II) OR HDMI)
L33 16 SEA ABB=ON PLU=ON L32 AND ?CRYST?
L34 14 DUP REM L33 (2 DUPLICATES REMOVED)
 D 1-14 IBIB ABS

FILE 'HOME' ENTERED AT 14:56:20 ON 19 OCT 2007
D QUE L3
D QUE L8

FILE HOME

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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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FILE LAST UPDATED: 18 Oct 2007 (20071018/UP). FILE COVERS 1950 TO DA

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FROM JANUARY 1926 TO DATE.

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FILE EMBASE
FILE COVERS 1974 TO 18 Oct 2007 (20071018/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE MARPAT

FILE CONTENT: 1961-PRESENT VOL 147 ISS 16 (20071012/ED)

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| DE | 102006007895 | 30 AUG 2007 |
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| JP | 2007221039 | 30 AUG 2007 |
| WO | 2007101371 | 13 SEP 2007 |
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| CA | 2537669 | 24 AUG 2007 |

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FILE LAST UPDATED: 18 OCT 2007 <20071018/UP>

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